Yang-Lee and Fisher Zeros of Multisite Interaction Ising Models on the Cayley-type Lattices

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Abstract

A general analytical formula for recurrence relations of multisite interaction Ising models in an external magnetic field on the Cayley-type lattices is derived. Using the theory of complex analytical dynamics on the Riemann sphere, a numerical algorithm to obtain Yang-Lee and Fisher zeros of the models is developed. It is shown that the sets of Yang-Lee and Fisher zeros are almost always fractals, that could be associated with Mandelbrot-like sets on the complex magnetic field and temperature planes respectively.

1 Introduction

In 1952, Lee and Yang in their famous papers [1] first proposed a new and effective method for investigation of phase transitions. They studied the distribution of zeros of the partition function considered as a function of a complex magnetic field (fugacity), and proved the circle theorem, which states that the zeros of the partition function of Ising ferromagnet lie on the unit circle in the complex fugacity plane (*Yang-Lee zeros*). After these pioneer works of Lee and Yang, Fisher [2], in 1964, initiated the study of partition function zeros in the complex temperature plane (*Fisher zeros*). These methods are then extended to other type of interactions and were widely applied [3]. Recently, Binek [4] showed that the density of Yang-Lee zeros can be determined experimentally from the field dependence of the isothermal magnetization data. The fractal structure of Fisher zeros in q-state Potts model on the diamond lattice was obtained by Derrida, Seze and Itzykson [5]. They showed that the Fisher zeros in hierarchical lattice models are just the Julia set corresponding to the renormalization transformation. Bosco and Goulard Rosa [6] investigated Yang-Lee zeros of the ferromagnetic Ising Model on the Cayley tree and associated these with the Julia set of the Cayley tree recursion map. They studied the case when the complex magnetic field was applied only to spins on lattice surface and found that Yang-Lee zeros are distributed along the unit circle.

The lattice models with multisite interaction Ising and Heisenberg models have been used for modelling the physical systems such as the binary alloys [8], classical fluids [9], liquid bilayers [11], solid ^3He [10], rare gases [12] and anisotropic magnets ($CeBi$, $EuSe$, etc.). These systems have rather complicated phase diagrams and unusual properties. Indeed, the Monte

Carlo results give evidence of the presence of phase transitions at nonzero values of the magnetic field for a number of ferromagnetic multisite interaction models [13]. There are few analytical results for these systems due to their greater complexity. Here we proposed a numerical algorithm for investigation of complex zeros of partition functions of models on the Cayley-type lattices.

This Letter is organized as follows. In Section 2 we give the model and derive the generalized recurrence equation. In Section 3 it is shown that the zeros of partition function can be associated with the set of external parameters (kT, *magnetic field*) at which the recurrence function has neutral periodic cycles. In Section 4 we present some definitions and theorems from complex analytic dynamics and give the numerical algorithm for obtaining Yang-Lee and Fisher zeros of the models. In the last section we give the explanation of the results and make conclusions.

2 The Model

We consider a multisite interaction Ising model on the Cayley-type lattice. The Cayley tree and Husimi lattice are the well known representatives of this class of recurrence lattices. In general, the Cayley-type lattice is constructed of p-polygons. It is characterized by p, the number of edges (the number of sites) of the polygon ($p = 2$ - usual Cayley tree, $p = 3$ - Husimi lattice) and by q, the number of p-polygons that go out from each site (Fig.1).

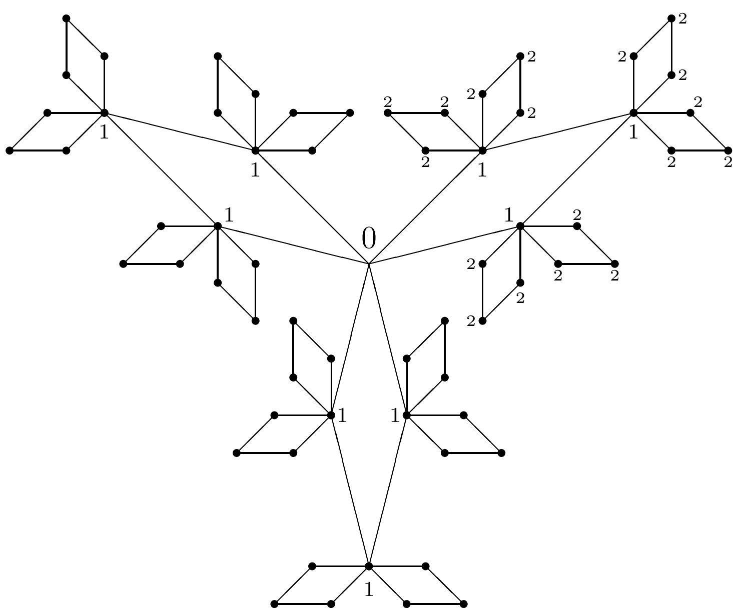

Fig. 1. The recursive structure of 4-polygon Cayley-type lattice with $q = 3$. The numbers $0, 1, 2$ stand for shells.

One of the pecular properties of the Cayley-type lattice is that in the thermodynamical limit (the number of shells are tended to ∞) the number of surface sites becomes proportional

to the number of inner sites of the lattice (for more detailes see [14, 15]). Therefore, the models defined on the Cayley-type lattice exhibit quite unusual behavior [16]-[18]. In the infinite dimensional Euclidean space the Cayley-type lattices are usually viewed as ramified trees with constant vertex connectivity. However, these can be embedded in the two-dimensional space of constant negative curvature (the hyperbolic plane) with fixed bond angles and length [7].

The Hamiltonian of the multisite interaction Ising model on a p-polygon Cayley-type lattice has the form

$$\mathcal{H} = -J_p' \sum_{\langle polygons\rangle} \prod S_p - h' \sum_i S_i, \tag{1}$$

where S_i takes on values ± 1, the first sum goes over all the p-polygons of the lattice and $\prod$ is the product of all spins on a p-polygon; the second sum goes over all the sites on the lattice.

The Cayley-type lattice has the advantage that for models defined on it one can derive the exact recurrence relation and use the theory of dynamical systems for investigation thermodynamical properties of the models [14]. Let us denote the statistical weight of the n-th generation branch with the basic spin at the state S as $g_n(S)$. By cutting of the n-th generation branch at the basic p-polygon one obtains $(q-1)(p-1)$ interacting $(n-1)$-th generation branches

$$g_n(S_0) = \sum_{S_1,\ldots,S_{p-1}} w(S_0, S_1, \ldots, S_{p-1}) g_n^\gamma(S_1) \cdots g_n^\gamma(S_{p-1}), \tag{2}$$

where $S_0, S_1, \ldots, S_{p-1}$ are the spins on the basic p-polygon, $\gamma = q-1$ and $w(S_0, S_1, \ldots, S_{p-1})$ is the statistical weight of the basic p-polygon

$$w(S_0, \ldots, S_{p-1}) = exp\left[J_p \prod_{k=0}^{p-1} S_k + \frac{h}{q}\sum_{k=0}^{p-1} S_k\right] \tag{3}$$

where $J_p = J_p'/kT$, $h = h'/kT$. Cutting apart the lattice at the central site one can obtain for the partition function $Z = \sum e^{-\beta H}$ the following expression

$$Z_n = \sum_{S_0} g_n^q\left(S_0\right). \tag{4}$$

Using Eq.(2) and introducing an auxiliary quantity $x_n = g_n(+)/g_n(-)$, we can get the recurrence relation for x_n, and express the thermodynamic quantities such as the magnetization, the specific heat, the free energy etc., in terms of x_n [14].

$$x_{n+1} = \frac{\sum_{k=0}^{p-1} a_{k+1} C_{p-1}^k x_n^{k\gamma}}{\sum_{k=0}^{p-1} a_k C_{p-1}^k x_n^{k\gamma}} \tag{5}$$

where

$$a_k = w(\underbrace{+,\ldots,+}_{k}, \underbrace{-,\ldots,-}_{p-k}) = \exp\left[(-1)^{p-k} J_p + \frac{2k-p}{q} h\right], \tag{6}$$

and $C_p^k = p!/(k!(p-k)!)$ is the simple combinations of p elements taken k at a time. Using the binomial theorem, one can obtain after some calculations the following general formula for the

recurrence relation of the multisite interaction Ising model on p-polygon Cayley-type lattice in an external magnetic field $x_{n+1} = f(x_n)$, where

$$f(x) = \frac{(e^{2h}x^{q-1}+1)^{p-1} + \tanh J_p(e^{2h}x^{q-1}-1)^{p-1}}{(e^{2h}x^{q-1}+1)^{p-1} - \tanh J_p(e^{2h}x^{q-1}-1)^{p-1}}. \tag{7}$$

Here we used the substitution $x_k \to e^{\frac{2h}{q}} x_k$.

In the following we shall use some definitions from the theory of dynamical systems. For every x_0 on the Riemann sphere ($x_0 \in \overline{C}$) $x_{n+1} = f(x_n)$, $n = 0, 1, 2, \ldots$, generates the forward orbit of x_0, which is denoted by $Or^+(x_0)$. If $x_n = x^*$ for some n in $Or^+(x^*)$ we say that x^* is a periodic point, and $Or^+(x^*)$ is called a periodic orbit or periodic cycle. If n is the smallest integer with that property, then n is the period of the cycle. Usually, if $n = 1$, x^* is called a fixed point. Obviously, x^* is a fixed point of f^n, if x^* is a periodic point of period n. (One should not confuse the iterations of f with the powers of f, i.e. $f^n = f \circ \ldots \circ f$ is different from $[f(x)]^n$). To characterize the stability of a periodic point x^* of period n we have to compute the derivatives. The complex number $\lambda = (f^n)'(x^*)$ $\left(' = \frac{d}{dx}\right)$ is called the eigenvalue of x^*. Using the chain rule of differentiation we see that this number is the same for each point in a cycle. A periodic point x^* is called (1) attracting (stable) if $|\lambda| < 1$, (superattracting if $\lambda = 0$), (2) repelling if $|\lambda| > 1$, (3) rationally neutral (indifferent) if $|\lambda| = 1$ and $\lambda^n = 1$ for some integer n, (4) irrationally neutral if $|\lambda| = 1$, but λ^n is never 1.

3 Zeros of the Partition Function and Neutral Periodic Cycles

Let us now consider the partition function of the model

$$Z_n \sim g_n^q(-)(e^{2h}x_n^q + 1) \equiv g_n^q(-)(e^{2h}\left[f^n(x_0)\right]^q + 1), \tag{8}$$

where $g_n(-)$ is an analytic function and $g_n(-) \neq 0, \infty$ for any kT, h and n; x_0 is an initial point of iterations ($x_0 = 1$ corresponds to the free boundary condition). From Eq.(8) one can see that Z_n is a rational function and the free energy of the system has the form

$$\mathcal{F} = -kT \lim_{n\to\infty} \ln Z_n = -kT \lim_{n\to\infty} \ln \left[g_n^q(-)\frac{P_n(z,\mu)}{Q_n^q(z,\mu)} \right], \tag{9}$$

where $P_n(z,\mu)$ and $Q_n(z,\mu)$ are polynomials in $z = e^{2J_p}$ and $\mu = e^{2h}$, where all coefficients are positive (see Eq.(5)). Since $g_n(-)$ is an analytic function, the free energy $\mathcal{F}$ has a singularity if and only if $P_n(z,\mu) = 0$ or $Q_n(z,\mu) = 0$. It is obvious from Eq.(8) and Eq.(9) that $Q_n(z,\mu)$ is the denominator of $f^n(x_0)$ function. Since ∞ cannot be a periodical point for $f(x)$ function, the condition $Q_n(z,\mu) = 0$ will not produce singularity of the free energy $\mathcal{F}$ in the thermodynamical limit. Hence, the singularities of $\mathcal{F}$ (phase transition points) correspond to zeros of the partition function Z_n ($P_n(z,\mu) = 0$), i.e. Yang-Lee or Fisher zeros [1, 2].

Let us now consider the problem of phase transitions on the Cayley-type lattices in terms of recurrence relations and dynamical systems theory. At high temperatures $T > T^*$ (T^* is the paramagnetic phase transition point) the recurrence relation has only one stable fixed point

x^*, corresponding to the paramagnetic phase. When the temperature is lowered, two different scenarios occur depending on the type of interactions. For ferromagnetic interactions ($J_p > 0$) at $T < T^*$ the "paramagnetic" fixed point either becomes unstable and there arise two different attracting fixed points, each corresponding to one of the two ferromagnetic phases with opposite directions of magnetization [15], or the "paramagnetic" fixed point remains stable and there arise an additional attracting fixed point (See Fig. 2 (d)). For antiferromagnetic interactions ($J_p < 0$) the "paramagnetic" fixed point at $T < T^*$ becomes unstable and there occur a period doubling bifurcation cascade and even chaos [19]. One says that for given external parameters (kT, h) the system is in the stable equilibrium state when the iterations of $f(x)$ approach a stable (attracting) k-cycle, and the system undergoes phase transition when, by changing the external parameters, the iterations of $f(x)$ pass from one (nonstable) k-cycle to the other (stable) k'-cycle (phase transitions between the modulated phases [20]). The values of external parameters at which the phase transition occurs may be obtained from the following conditions

$$f^k(x) = x, \qquad |(f^k)'(x)| = 1.$$

We see that the phase transition points could be associated with neutral periodic cycles of the mapping. We call the set of parameter values, at which the rational function f from Eq.(7) has neutral periodic cycles, the Mandelbrot-like set of f. Thus, to investigate the Yang-Lee and Fisher zeros one can study the Mandelbrot-like sets of f.

4 Mathematical Background and the Numerical Algorithm

In this section we give the required definitions and theorems from complex analytic dynamics on the Riemann sphere [21, 22] and develop a numerical algorithm for obtaining the Yang-Lee and Fisher zeros of the model.

One can consider any rational function $f(x) = P(x)/Q(x)$, where $P(x)$ and $Q(x)$ are polynomials in x as an holomorphic map on a Riemann sphere. The poles of the rational function are simply the points of Riemann sphere $\overline{C} = C \bigcup \{\infty\}$, that are mapped to ∞ (the upper pole of the Riemann sphere). The degree of $f(x)$ $d = \deg(f)$ is defined as

$$d = \max\{\deg(P), \deg(Q)\}.$$

Also, the degree of f is the number (counted with multiplicity) of inverse images of any point of $\overline{C}$. v is a critical value of f if the equation $f(c) = v$ has a solution the multiplicity of which is greater than one. Such a solution c is called a critical point. In local coordinates this is equivalent to the condition $f'(c) = 0$ (at least when $c \neq \infty$). To discuss the behavior of $f(x)$ near ∞ one usually invokes another transformation, the reflection $r(x) = 1/x$ at the unit circle, which exchanges 0 with ∞; i.e. to treat the behavior of $f(x)$ near ∞, one is to consider $\varphi(x) = r(f(r(x))) = r \circ R \circ r(x)$ in the vicinity of 0. Below we give some theorems from complex analytic dynamics without proofs. The reader should consult Carleson and Gamelin [21] for proofs.

Theorem 1. The number of critical points of f is at most $2d - 2$.

If x^* is an attracting fixed point for f, we define the basin of attraction of x^*, denoted by $A(x^*)$, to consist of all x such that $f^n(x^*)$ is defined for all $n \geq 1$ and $f^n(x) \to x^*$. The

connected component of $A(x^*)$ containing x^* is called the immediate basin of attraction of x^* and is denoted by $A^*(x^*)$. If γ is an attracting cycle of period n, then each of the fixed points of $f^n(x^*)$ has its basin and $A(\gamma)$ is simply the union of these basins.

Theorem 2. If x^* is an attracting periodic point, then the immediate basin of attraction $A^*(x^*)$ contains at least one critical point.

Theorem 3. If x^* is a rationally neutral periodic point, then each immediate basin of attraction associated with the cycle of x^* contains a critical point.

Theorem 4. The total number of attracting and neutral cycles is at most $2d-2$.

The numerical algorithm is based on Theorems 1-4 and the well known fact that the convergence of iterations to neutral periodic cycle is very weak; i.e. one has to make a number of iterations (infinite number of iterations) in order to approach the neutral periodic cycle. Of course, the initial point does not belong to the periodic cycle or the Julia set of mapping (for the definition of the Julia set see Ref. [21]). The algorithm is as follows: One finds all the critical points of the mapping and investigates the convergence of all the orbits of critical points (critical orbits) to any attracting periodic cycle. If all critical orbits converge, for example, after n iterations, one says that the system is in stable equilibrium state, otherwise the system undergoes phase transition. Of course, the last statement is not rigorous since a weak convergence to an attracting periodic cycle is possible. Depending on the choice of n and ε - the accuracy of approaching the attracting cycle, the phase transition pictures may change. Our complutergraphical experiments showed that $n = 700$ and $\varepsilon = 10^{-4}$ are optimal values for n and ε, and the pictures generated by this algorithm will not qualitatively change when n is increased and/or ε decreased from their optimal values. In our algorithm we supposed that the cases where neutral periodic cycles are irrational are very rare and negligible.

5 Results and Pictures

One can easily find all the critical points of mapping f from Eq.(7) as is described in the previous section. The critical points are as follows: $x = 0$ with multiplicity $q-2$, $x = \infty$ with multiplicity $q-2$ and $2(q-1)(p-1)$ solutions of equations $(e^{2h}x^{q-1}+1)^{p-1} = 0$ and $(e^{2h}x^{q-1}-1)^{p-1} = 0$. The degree of our mapping f is $d = (p-1)(q-1)$ and, according to Theorem 1 of Section 4, these all are critical points of f. One can easily find that the most of the critical orbits after the first iteration are intersected and can consider only the orbits starting at points 0, z ($\infty \to z$), 1, -1 for $p > 2$ and $1/z$, z for $p = 2$. Also, the orbits of 0 and ∞ intersect when p is odd and the orbits of 1 and -1 intersect when q is odd. Bellow we give some pictures generated by our algorithm. Fig. 2 shows computergraphical study for Fisher zeros of the Ising model on the Cayley tree ($p = 2$, $q = 3$) for $J' = 1$ and different values of magnetic field h'. We have experimental evidence that all critical orbits converge in white regions. Physical phase transitions take place at the points where black regions intersect the real axis. We see that for $h' = 0$ (Fig. 2 (a)) the second order phase transition occurs for $z = 3$ in accordance with Baxter's result [15] and for $h' = 1$ (Fig. 2 (c)) there is no phase transition for $kT > 0$. For $h' = 0.5$ (Fig. 2 (b)) the first order phase transition occurs in "*cat face*"-like region. Figure 2 (d) shows the neutral fixed point of $f(x)$ function corresponding to phase transition in the "*cat face*"-like region of Fig. 2 (b). A care should be taken in calculations for small $kT < 0.07$ because one of the attracting fixed points tends to infinity when the temperature is lowered.

Since the free energy of the Ising model on the Cayley tree is an even function of h', Figs. 2 (a)-(c) are invariant under the transformation $h' \to -h'$ and show phase transitions for both ferromagnetic and antiferromagnetic interactions ($kT \to -kT$ is equivalent to $J' \to -J'$ and $h' \to -h'$). In Fig. 3 we present Yang-Lee zeros of the ferromagnetic Ising model on the Cayley tree. Figs. 3 (a)-(b) show that the phase transition exists at positive temperatures for $h' = 0.5$ and $h' = -0.5$ in accordance with Fig. 2(b). The set of Yang-Lee zeros at the critical point $z = 3$ is shown on Fig. 3(c). One can see that in this case a real phase transition occurs at zero magnetic field only as in usual ferromagnetic systems. It is interesting to note that the set of Yang-Lee zeros of ferromagnetic Ising model on the Cayley tree resembles the boundary of the Mandelbrot set of the quadratic mapping $z \to z^2 + c$. In this case the Yang-Lee zeros are not located on the unit circle because in the thermodynamical limit the contribution of surface and inner spins to the partition function of the model on Cayley tree are of the same order. In Fig. 3 (d) we give the improved set of Fisher zeros of Ising model on the Husimi lattice ($p = 3$, $q = 4$) previously obtained in Ref. [23].

In conclusion, we should like to note that the numerical algorithm presented in this Letter may be applied for obtaining Yang-Lee and Fisher zeros of any model on the Cayley-type lattice, for which one-dimensional recurrence relation can be derived. It is remarkable that there appear the well-known Mandelbrot set figures. This phenomenon is known as the universality of the Mandelbrot set [24].

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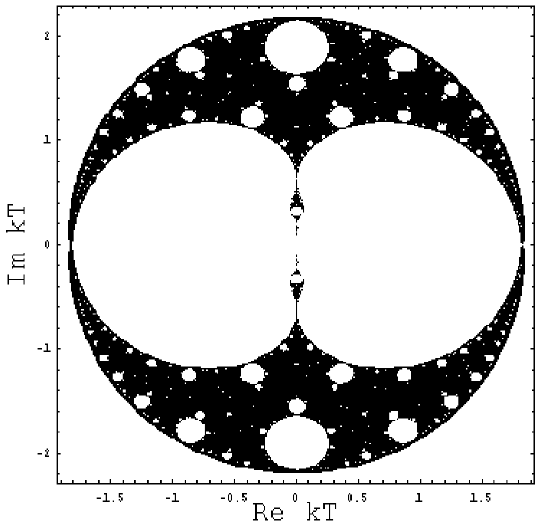
Figure Caption

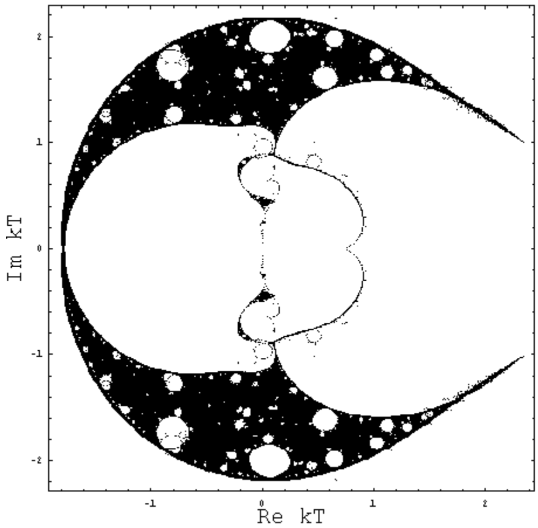
Figure 1. The recursive structure of 4-polygon Cayley-type lattice with $q = 3$. The numbers $0, 1, 2$ stand for shells.

Figure 2. The Fisher zeros of Ising model on the Cayley tree. (a) $J' = 1$, $h' = 0$; (b) $J' = 1$, $h' = 0.5$; (c) $J' = 1$, $h' = 1$; (d) The plot of $f(x)$ function from Eq. (7) corresponds to the phase transition point $kT = 0.7256$, $J' = 1$, $h' = 0.5$ of (b).

Figure 3. (a)-(c) The Yang-Lee zeros of Ising models on the Cayley tree; (a) $p = 2$, $q = 3$, $z = 15, 742$; (b) a close up from left; it is noteworthy that the set in question may be obtained by mapping $r(\mu) = 1/\mu$ from the Mandelbrot set boundary of (a); (c) $p = 2$, $q = 3$, $z = 3$; (d) The Fisher zeros of multisite interaction Ising model on Husimi lattice $J' = -1$, $h' = 3$, $p = 3$, $q = 4$.



(a)



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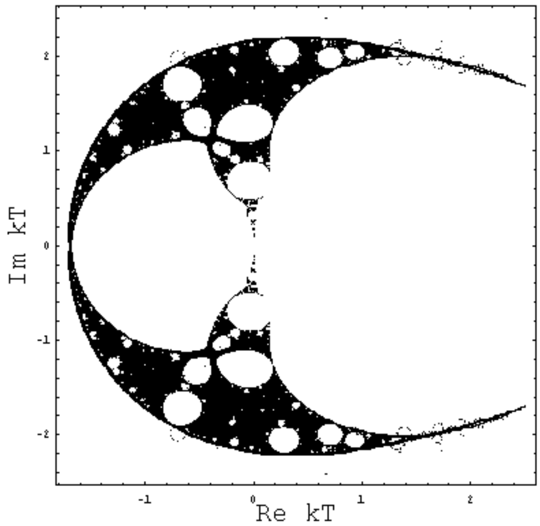

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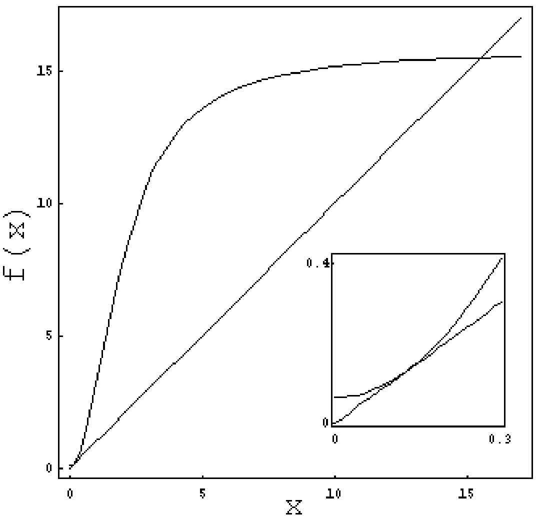

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Figure 2

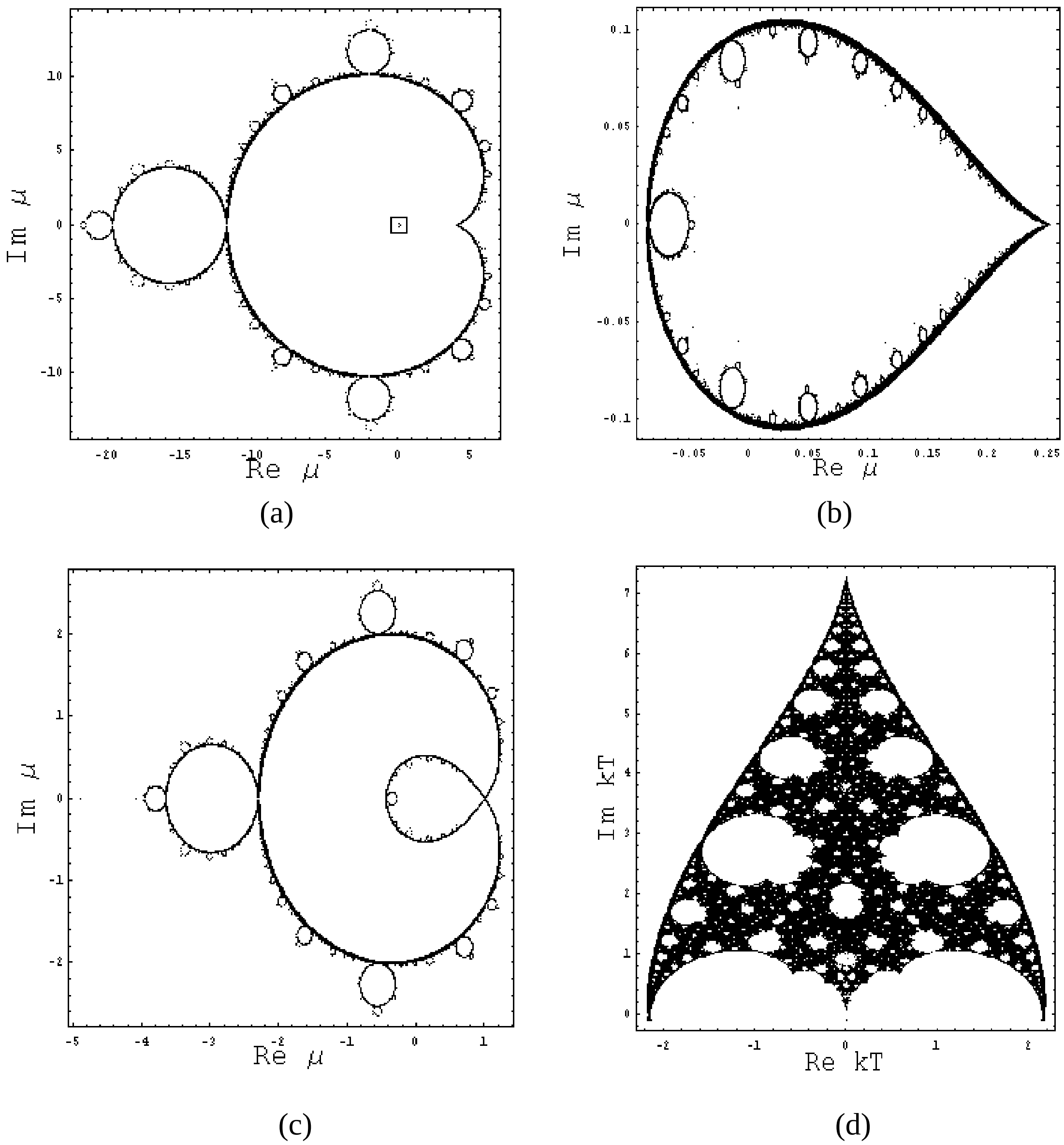

Figure 3